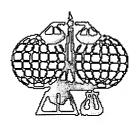
# **APPENDIX A**

Taken from:

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Fused Ring Nor	Fused Ring Nomenclature Phane Nomenclatur		ıre	Phane Nomenclature Part II NEW	
Glossary of T Bioinorganic (		Glossary of Medicinal Chemistry Terms		Nomenclature of Isotopically Modified Compounds (Section H)	
and <u>Periodi</u> (1999 table p	IUPAC Atomic Weights and Periodic Table (1999 table plus 2001 proposals) New Values			Spiro nomenclature	
Natural pr nomenclature (	4	Radicals, Ions & Radical Ion Nomenclature	2	Gold Book IUPAC definitions of terms.	

Numerical Terms to

Fullerene nomenclature

NEW 9999 Watch this space!

Recommendations by IUPAC and IUBMB (International Union of Biochemistry and Molecular Biology) from the Joint Commission on Biochemical Nomenclature

Nomenclature of Amino Acids Nucleic Acid & Constituents Carbohydrate and Peptides Abbreviations and Symbols Nomenclature Conformation of Polypeptide **Conformations of** Conformation of Chains Polysaccharide Chains Polynucleotide Chains Glycopeptide, Glycoprotein & Glycolipid Nomenclature Cyclitol Nomenclature Peptidoglycan Nomenclature Polymerised Amino Acids Newsletter (1996 & Lipid Nomenclature Nomenclature 1999) Prenol Nomenclature Vitamin D Steroid Nomenclature Terpenoid precursors Nomenclature Retinoid Nomenclature Folic Acid Nomenclature Carotenoid Nomenclature (Vitamin A) Corrinoid Tocopherol Nomenclature Vitamin B-6 Nomenclature Nomenclature (Vitamin E) (Pyridoxal) (Vitamin B-12) **Biochemical Phosphorus** Lignan Nomenclature **Biochemical Thermodynamics** NEW Compounds Nomenclature of Quinones with Tetrapyrrole Nomenclature Watch this space! Isoprenoid Chains NEW NEW

Other recommendations, bibliographic data etc.

| Nomenclature Nucleic Acid | Sequences | (incompletely specified | bases) | Enzyme Nomenclature | (EC 1 oxidoreductases, EC 2 transferases, EC 3 hydrolases, EC 4 lyases, EC 5 isomerases and EC 6 ligases) and Supplements 1 to 8 |

| Electron Transport | Peptide Hormone | Proteins Nomenclature | Nomenclature | Enzyme kinetics | Enzyme

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nomenclature recommendations	Organic Chemical Nomenclature	IUBMB Biochemical Nomenclature
Bibliography of IUPAC Nomenclature Books	Bibliography of IUPAC Macromolecular Chemical Nomenclature	Bibliography of IUPAC Inorganic Chemical Nomenclature
IUPAC Spectrochemical recommendations (mirror sites in USA, Germany, Japan, Korea, South Africa, UK)	Pure and Applied Chemistry; contents (mirror sites in USA, Germany, Japan, Korea, South Africa, UK) also some text and PDF files	Chemistry International; contents (mirror sites in USA, Germany, Japan, Korea, South Africa, UK) also PDF file of text
Parameters and Symbols for NMR (mirror sites in <u>USA</u> , <u>Germany</u> , <u>Japan</u> , <u>Korea</u> , <u>South Africa</u> , <u>UK</u> )	IUPAC Organisation and people (mirror sites in <u>USA</u> , <u>Germany</u> , <u>Japan</u> , <u>Korea</u> , <u>South</u> <u>Africa</u> , <u>UK</u> )	IUPAC Publications (mirror sites in <u>USA</u> , <u>Germany</u> , <u>Japan</u> , <u>Korea</u> , <u>South Africa</u> , <u>UK</u> )
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- Subscripts e.g. ethanol C<sub>2</sub>H<sub>5</sub>OH
- Superscripts e.g. sodium chloride Na<sup>+</sup>Cl<sup>-</sup>
- Greek, etc e.g. α-amino acid (graphic Greek) or α-amino acid (using symbol)

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## IUPAC-IUB Commission on Biochemical Nomenclature (CBN)

## Nomenclature of Lipids

Recommendations, 1976

http://www.chem.qmul.ac.uk/iupac/lipid/

World Wide Web version Prepared by G. P. Moss

Department of Chemistry, Queen Mary University of London, Mile End Road, London, E1 4NS, UK g.p.moss@qmul.ac.uk

These Rules are as close as possible to the published version prepared by the Working Group on Lipid Nomenclature: H. Hirschmann (U.S.A.), P. Karlson (Federal Republic of Germany; convenor), W. Stoffel (Federal Republic of Germany), F. Snyder (U.S.A.), S. Veibel (Denmark), F. Vögtle (Federal Republic of Germany) and the Working Group on Glycolipid Nomenclature: S. Basu (U.S.A.), R. O. Brady (U.S.A.), R. M. Burton (U.S.A.), R. Caputto (Argentina), S. Gatt (Israel), S. I. Hakomori (U.S.A.), M. Philippart (U.S.A.), L. Svennerholm (Sweden), D. Shapiro (Israel), C. C. Sweeley (U.S.A.), H. Wiegandt (Federal Republic of Germany; convenor) [see *Biochem. J.*, 1978, 171, 21-35; *Chem. Phys. Lipids*, 1978, 21, 159-173; *Eur. J. Biochem.*, 1977, 79, 11-21; *Hoppe-Seyler's Z. Physiol. Chem.*, 1977, 358, 617-631; *J. Lipid Res.*, 1978, 19, 114-128; *Lipids*, 1977, 12, 455-468; *Mol. Cell. Biochem.*, 1977, 17, 157-171; *Biochemical Nomenclature and Related Documents*, 2nd edition, Portland Press, 1992, pages 180-190. Copyright IUPAC and IUBMB; reproduced with the permission of IUPAC and IUBMB]. If you need to cite these rules please quote these references as their source.

Any comments should be sent to any member of the Committee.

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#### Introduction

In 1967, a 'Document for Discussion' on lipid nomenclature [1] was issued by CBN. It included a special system for the designation of configuration in glycerol derivatives that deviated considerably from standard stereochemical nomenclature. This system is based upon a fixed numbering ('stereospecific numbering') for glycerol, regardless of substituents. It was hoped [1] that 'discussion will lead shortly to the formulation' of recommendations acceptable to chemists in the field of lipids.

In subsequent years, there has been little discussion about this principle of stereospecific numbering; it has been well-accepted within the field of glycerol derivatives, for which it has been especially useful and is widely used. However, during this same period, many new and complex lipids and glycolipids have been isolated. Moreover, the Commissions on the Nomenclature of Organic Chemistry (CNOC) and Inorganic Chemistry (CNIC) issued, in 1973, *Nomenclature of Organic Chemistry, Section D* [2], which includes a section on the nomenclature of phosphorus-containing organic compounds and necessitates a reconsideration of the earlier nomenclature [1] in this area.

Note. CBN does not wish to imply that the idea of stereospecific numbering should be applied to other groups of compounds. it is the symmetry of glycerol itself, but the asymmetry of its derivatives carrying different substituents at O-1 and O-3, as well as the unique place of these compounds in lipid metabolism, that makes this special treatment desirable.

The present 'Recommendations 1976' are based on reports of working groups on lipids and glycolipids. The main features are:

- (a) the system of stereospecific numbering is retained;
- (b) semisystematic nomenclature is extended to the plasmalogens;
- (c) a semisystematic nomenclature for higher glycosphingolipids, based on trivial names for specific triand tetrasaccharides, is proposed.

#### Partial update

Since the preparation of this report the Nomenclature of Glycolipids, Recommendations 1997, have been published [see Adv. Carbohydr. Chem. Biochem. 1999, 55, in press; Carbohydr. Res., 1998, 312, 167-175; Eur. J. Biochem., 1998, 257, 293-298; Glycoconjugate J., 1999, 16, 1-6; J. Mol. Biol., 1999, 286, 963-970; Pure Appl. Chem., 1997, 69, 2475-2487]. These supercede parts of this document.

#### References for this section

- 1. IUPAC-IUB Commission on Biochemical Nomenclature (1967) Eur. J. Biochem. 2, 127-131, also 12, 1 (1970); [see also Biochemistry, 1967, 6, 3287-3292; Biochem. J., 1967, 105, 897-902; J. Biol. Chem., 1967, 242, 4845-4849; Hoppe-Seyler's Z. Physiol. Chem., 1969, 350, 279-285 (on German)].
- 2. International Union of Pure and Applied Chemistry (1973) *Information Bulletin*, Appendix 31. [See also *Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F, and H*, Pergamon Press, 1979. Edited by J Rigaudy and S P Klesney.]

Continued with Lip 1 and Lip 2. Fatty acids, neutral fats, long-chain alcohols and long-chain bases Return to IUPAC Chemical Nomenclature home page.





## Recommendations Lip-1 and Lip-2

#### Continued from Introduction

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  - B. Individual compounds (Lip-2.11 to Lip-2.12)

#### I. FATTY ACID, NEUTRAL FATS, LONG-CHAIN ALCOHOLS AND LONG-CHAIN BASES

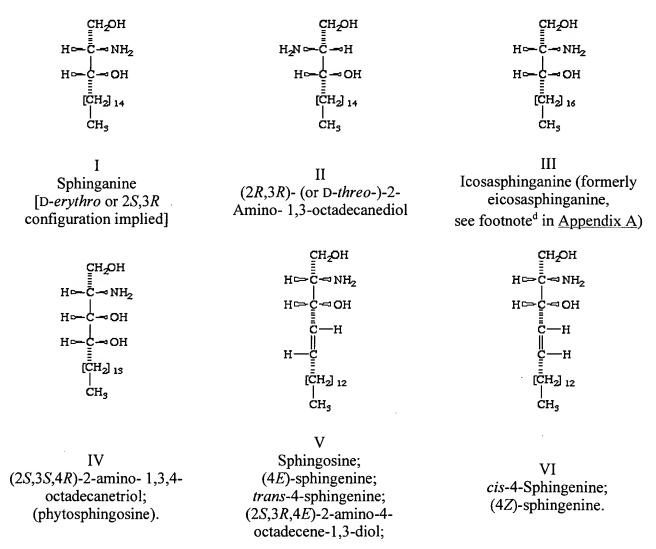
#### A. Generic Terms

- Lip-1.1. The term 'fatty acid' designates any one of the aliphatic monocarboxylic acids that can be liberated by hydrolysis from naturally occuring fats and oils. In the terms 'free fatty acids' or 'nonesterified fatty acids', now widely in use, 'free' and 'nonesterified' are actually redundant and should be omitted (See Lip-1.14). [The designation 'aliphatic carboxylate ( $C_{10}$ - $C_{26}$ , nonesterified)' used by the Commission on Quantities and Units in Clinical Chemistry is correct, but rather cumbersome.] Whenever the sum of fatty acids and their esters is determined by an analytical method, this should be explicitly stated. (See also Lip-1.6).
- Lip-1.2. 'Neutral fats' are mono-, di-, or triesters of glycerol with fatty acids, and are therefore termed monoacylglycerol, diacylglycerol, or triacylglycerol, as appropriate. 'Acylglycerols' includes mixtures of any or all of these.
- Comments. (a) The term 'acyl' is used in Organic Nomenclature [3] to denote the radical formed by loss of the OH group from the acid function of any acid (cf. Lip-1.6). We are concerned here with acyl radicals of aliphatic carboxylic acids with four or more carbon atoms, the larger members of which (>  $C_{10}$ ) are also known as 'higher fatty acids'.
- (b) The old terms monoglyceride, diglyceride, and triglyceride are discouraged and should progressively be abandoned, not only for consistency, but mainly because strict interpretation does not convey the intended meaning. 'Triglyceride', taken literally, indicates three glycerol residues (e.g., cardiolipin),

diglyceride two (e.g., phosphatidyIglycerol), and a monoglyceride is a monoacy1glycerol.

**Lip-1.3.** The generic term 'long-chain alcohol' or 'fatty alcohol' refers to an aliphatic compound with a chain-length greater than  $C_{10}$  that possesses a terminal  $CH_2OH$  group. Such alcohols should be named according to systematic nomenclature [3]. (See <u>Lip-1.7</u>).

Lip-1.4. The term 'sphingoid' or 'sphingoid base' refers to sphinganine (cf. Lip-1.8), [D-erythro-2-amino-1,3-octadecanediol (I)], to its homologs and stereoisomers (II, III), and to the hydroxy and unsaturated derivatives of these compounds (IV-VI). The term 'long-chain base' may be used in a wider sense to indicate any base containing a long-chain aliphatic radical.



Lip-1.5. The following generic terms are used for the following groups of compounds:

- (a) sphingolipid, for any lipid containing a sphingoid;
- (b) ceramide, for an N-acylated sphingoid;
- (c) sphingomyelin, for a ceramide-1-phosphocholine. (See [2] for this use of 'phospho'; also Lip-2.11):
- (d) *glycosphingolipid*, for any lipid containing a sphingoid and one or more sugars. (See below for other generic terms).

#### **B.** Individual Compounds

#### 1. Fatty Acids and Alcohols

Lip-1.6. Fatty acids (cf. Lip-1.1) and their acyl radicals (cf. Lip-1.2, comment [a]) are named according to the IUPAC Rules for the Nomenclature of Organic Chemistry ([3], Rule C-4). (A list of trivial names is given in Appendix A.) Fatty acids are numbered with the carbon atom of the carboxyl group as C-1. By standard biochemical convention, the ending '-ate' in, e.g., palmitate denotes any mixture of the free acid and its ionized form in which the cations are not specified. The ending '-ate' is also used to designate esters, e.g., cholesteryl palmitate, ethylidene dilaurate, etc. (cf. Lip-1.12). Structural isomers of polyunsaturated acids, hitherto distinguished by Greek letters (e.g., α- and γ-linolenic acids), are better distinguished by the locants of the unsaturated linkages [e.g. (9,12,15)- and (6,9,12)-linolenic acids, respectively]. (See Lip-1.15). However, the Greek letter prefixes may be useful in (defined) abbreviations (see Appendix A).

Lip-1.7. Long-chain alcohols (fatty alcohols) and the radicals derived from them should be designated by their systematic names ([3], Rules C-201 and A-1 et seq.), but not by trivial names that are derived from those of fatty acids.

#### Examples:

- (a) 1-hexadecanol and hexadecyl-, not palmityl alcohol and palmityl-;
- (b) 1-dodecanol and dodecyl-, not lauryl alcohol and lauryl-.

#### 2. Sphinganine and Derivatives

Lip-1.8. The compound previously known as dihydrosphingosine [D-erythro-2-amino-1,3-octadecanediol or (2S,3R)-2-amino-1,3-octadecanediol] is called *sphinganine* (1).

**Lip-1.9.** Trivial names of higher or lower homologs of sphinganine may be derived by adding a prefix ([3], Rule A-1) denoting the total number of carbon atoms in the main chain of the homolog, e.g., icosasphinganine for the  $C_{20}$  compound (III), hexadecasphinganine for the  $C_{16}$  compound.

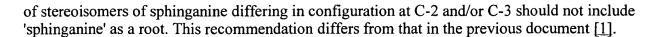
Note. See footnote d in Appendix A re 'icosa' for 'eicosa'.

Lip-1.10. The recommendations on the <u>Nomenclature of Glycolipids</u> imply that parts of Lip-1.10 are no longer recommended. The following version has a text edited to reflect current recommendations. Readers who wish to consult the original wording can see this as an <u>appendix</u>.

Affixes denoting substitution of sphinganine (hydroxy, oxo, methyl, etc.) are used as usual, according to existing rules [3]. The configuration is indicated using the R/S system [6].

Sphingoids differing from sphinganine in their configurations at C-2 and/or C-3 should be named not as derivatives of sphinganine, but with fully systematic names [3], using the prefixes D-threo, L-erythro, as appropriate, e.g., D-threo-2-amino-1,3-octadecanediol, or (2R,3R)-2-amino-1,3-octadecanediol, for II (cf. Rule Carb-8 in [5]). (Cf. Lip-1.11, example [d]).

Comments. (a) The semisystematic names for the sphingoids are significantly shorter than the fully systematic names only if the terms chosen imply not only substituents but also configurations. Therefore, the name 'sphinganine' specifies the D-erythro configuration, and it is logical that the names



(b) The configurational prefixes using the R/S system [6] may change with changes in the substitution. For example C-3 is R in icosasphinganine (III) but S in 4-hydroxysphinganine (IV).

#### Examples:

- (a) (2R,3R)-2-amino-1,3-octadecanediol, for II;
- (b) (2S,3S,4R)-2-amino-1,3,4-octadecanetriol for IV;
- (c) (2S,3R,4E)-2-amino-4-octadecene-1,3-diol for sphingosine (V) (See also Lip-1.11).

Lip-1.11. Names for unsaturated compounds are derived from the names of the corresponding saturated compounds by the appropriate infixes, namely ene, diene, yne, etc. [3]. If the geometry of the double bond is known, it should be indicated by the more modern *E-Z* system (cf. [6], Rule E-2.2), e.g., (4*E*)-sphingenine for sphingosine (V).

Comment. The trivial name 'sphingosine' (V) is retained. If trivial names other than sphingosine are used, they should be defined in each paper in terms of this nomenclature, or of the general nomenclature of organic chemistry [3].

Other names for compounds described in <u>Lip-1.10</u> and <u>Lip-1.11</u>:

- (a) omitted, see appendix;
- (b) (4E)-sphingenine for sphingosine (V);
- (c) (4Z)-sphingenine for the geometric isomer of sphingosine (VI);
- (d) D-threo-2-amino-1,3-octadecanediol for the C-2 epimer of sphinganine (II); cf. <u>Lip-1.10</u>, example (a).

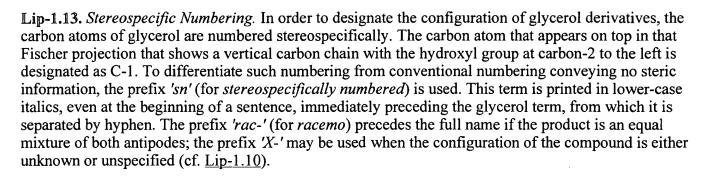
## 3. Glycerol Derivatives

**Lip-1.12.** Esters, ethers and other *O*-derivatives of glycerol are designated according to Carb-15 of the *Rules of Carbohydrate Nomenclature* [5], i.e. by a prefix, denoting the substituent, preceded by a locant. if the substitution is on a carbon atom, the compound is designated by its systematic name and not as a derivative of glycerol (e.g., 1,2,3-nonadecanetriol for  $C_{16}H_{33}$ CHOH-CHOH-CH<sub>2</sub>OH, which could be considered as 1-*C*-hexadecy1glycerol). It is permissible to omit the locant 'O' if the substitution is on the oxygen atoms of glycerol.

#### Examples:

- (a) tristearoylglycerol or tri-O-stearoyl glycerol or glycerol tristearate, or glyceryl tristearate;
- (b) 1,3-benzylideneglycerol or 1,3-O-benzylideneglycerol;
- (c) glycerol 2-phosphate (a permissible alternative to this term is 2-phosphoglycerol) [10].

Comment. The alternative system set forth in Carb-16 of the *Rules on Carbohydrate Nomenclature* [5], i.e. the use of the suffix '-ate', is less suitable for glycerol esters, with the exception of the phosphates (see Examples). However, this system may be used to designate esters of monofunctional alcohols, e.g. cholesteryl palmitate (cf. <u>Lip-1.6</u>).



#### Examples:

- (a) sn-glycerol 3-phosphate for the stereoisomer (VII = VIII), previously known as either L- $\alpha$ -glycerophosphate or as D-glycerol 1-phosphate;
- (b) rac-1-hexadecylglycerol;
- (c) 1,2-dipalmitoyl-3-stearoyl-X-glycerol.

CH\_OPO\_3H\_2

HO 
$$\subset$$
  $\subset$  H  $\equiv$  H  $\subset$   $\subset$  OH

CH\_OPO\_3H\_2

VII VIII

sn-Glycerol 3-phosphate

L-(glycerol 3-phosphate) ≡ D-(glycerol 1-phosphate)

Comments. (a) The problem of distinguishing between stereoisomers was discussed *in extenso* in the 1967 document [1]. In brief, difficulties arise because glycerol is a prochiral compound. The parent substance of many phospholipids, natural glycerol phosphate, has been named both as L-α-glycerol phosphate [7] (VII) and, according to standard rules of nomenclature, D-glycerol 1-phosphate [8] (VIII). When the *R/S* system (sequence rule) is applied, substitution of one of the primary hydroxyl groups often leads to changes in the configurational prefix, thus obscuring chemical and biogenetical relationships; it is generally inapplicable to the steric description of such mixtures as occur in triacylglycerols isolated from natural sources. The stereospecific numbering of glycerol and its derivatives as proposed by Hirschmann [9], described above and in [1], avoids these difficulties; it has proved useful and is widely accepted.

(b) The enantiomer of *sn*-glycerol 3-phosphate (VII) is *sn*-glycerol 1-phosphate (IX), as is evident from the structures.

IX sn-Glycerol 1-phosphate [L-(glycerol 1-phosphate)] = D-(glycerol 3-phosphate)]

#### C. Symbols and Abbreviations

Lip-1.14. The term 'fatty acids' (cf. Lip-1.1) should not be abbreviated. The use of abbreviations like

'FFA' for 'free fatty acids' or 'NEFA' for 'non-esterified fatty acids' is strongly discouraged.

Comment. The words 'acids' and 'esters' serve to distinguish the 'free' (nonesterified) and 'bound' (esterified) fatty acids and are as short or shorter than the abbreviations themselves.

Lip-1.15. In tables and discussions where various fatty acids are involved, the notation giving the number of carbon atoms and of double bonds (separated by a colon) is acceptable, e.g. 16:0 for palmitic acid, 18:1 for oleic acid. Also, terms such as '(18:0)acyl' may be used to symbolize radicals of fatty acids. (See Appendix A).

Comment. This system is already widely used. It should, however, be kept in mind that it sometimes does not completely specify the fatty acid. For example,  $\alpha$ -linolenic acid and  $\gamma$ -linolenic acid are both 18:3 acids; the designation 18:3 is therefore ambiguous. In such a case, the position of double bonds shollid be indicated, e.g. 18:3(9,12,15) for (9,12,15)-linolenic acid, formerly known as  $\alpha$ -linolenic acid.

Lip-1.16. It is sometimes desirable (for example, in discussing the biosynthesis of lipids) to indicate the position of each double bond with reference not to the carboxyl group (always C-1), but to the end of the chain remote from the carboxyl. If n is the number of carbon atoms in the chain (i.e. the locant of the terminal methyl group) and x is the (lower) locant of the double bond, the position of the double bond may be defined as (n minus x). Thus, the common position of the double bond in oleic and nervonic acids may be given as 18-9 and 24-9, respectively. This structural regularity should not be expressed as  $\omega$ 9.

Lip-1.17. The system described in <u>Lip-1.15</u> may also be used to denote alcohols and aldehydes related to fatty acids, provided that the nature of the residue is clearly indicated either by the appropriate name of the compound(s) (e.g. 18:1 alcohol) or in the heading of the table. The 1-ene of alk-1-en-1-yl (i.e. 1-alkenyl) compounds is not counted in this system (see <u>Lip-2.10</u>, comment).

Lip-1.18. For many complex lipids, a representation of the structures using symbols rather than structural formulae may be useful. Symbols proposed for various constituents are given in <u>Appendix B</u> (see also [10]), and, for glycolipids, in <u>Lip-3.13</u>. They are constructed in analogy to those in use for amino acids [11], nucleosides [12] and saccharides [13].

#### II. PHOSPHOLIPIDS

#### A. Generic Terms

The Rules of the *Nomenclature of Organic Phosphorus Compounds*, also known as D-Rules [2] recognize, for biochemical usage, the prefix 'phospho' as an alternate to '*O*-phosphono-' (or '*N*-phosphono-'). By a similar convention [10], '-phospho-' may be used as an infix to designate the phosphodiester bridge present in such compounds as glycerophosphocholine. The use of root names like 'phosphatidic acid' is retained and extended (Lip-2.3 to Lip-2.4).

Lip-2.1. 'Phospholipid' may be used for any lipid containing phosphoric acid as mono- or diester. Likewise, lipids containing C-phosphono groups (e.g. compound X) may be termed 'phosphonolipids'.

$$\begin{array}{ccc} CH_2O-CO-R' \\ \hline R"CO-O & C \rightarrow H & NH_2 \\ \hline & & | \\ CH_2O-PO(OH)-CH_2CH-CO_2H \end{array}$$

## X A phosphonolipid

Lip-2.2. 'Glycerophospholipid' signifies any derivative of glycerophosphoric acid that contains at least one O-acyl, or O-alky], or O-(1-alkenyl) group attached to the glycerol residue. Generic names for other classes of phospholipids may be coined according to this scheme, e.g., sphingophospholipid, inositolphospholipid.

Comment. The old terms, 'phosphatide', 'phosphoglyceride', and 'phosphoinositide' are no longer recommended because they do not convey the intended meaning (see also <u>Lip-1.2</u>).

Lip-2.3. 'Phosphatidic acid' signifies a derivative of a glycerol phosphate (glycerophosphate) in which both remaining hydroxyl groups of glycerol are esterified with fatty acids. The position of the phosphate group may be emphasized by stereospecific numbering.

Comment. For the most common (3-sn) phosphatidic acid and its derivatives, the locants are often omitted. However, 'phosphatidyl' without locants can lead to ambiguities. It is therefore preferable to use the proper locants, for example, 2-phosphatidic acid for compound XI, and 3-sn-phosphatidylserine for XIIa.

CH2O-CO-R'

H2O<sub>2</sub>P -O 
$$\stackrel{\circ}{\sim}$$
  $\stackrel{\circ}{\sim}$  H

 $\stackrel{\circ}{\sim}$  H

 $\stackrel{\circ}{\sim}$  H

 $\stackrel{\circ}{\sim}$  H

 $\stackrel{\circ}{\sim}$  XI

2-Phosphatidic acid

 $\stackrel{\circ}{\sim}$  CH2O-CO-R'

 $\stackrel{\circ}{\sim}$   $\stackrel{\circ}{\sim}$  H

 $\stackrel{\circ}{\sim}$  NH2

 $\stackrel{\circ}{\sim}$   $\stackrel{\circ}{\sim}$  NH2

 $\stackrel{\circ}{\sim}$  CH2O-PO(OH)-O-CH2CH-CO2H

XIIa

Phosphatidylserine

(3-sn-phosphatidylserine)

[See also entry from 1980 Newsletter]

Lip-2.4. The common glycerophospholipids are named as derivatives of <u>phosphatidic acid</u>, e.g. 3-sn-phosphatidylcholine (this term is preferred to the trivial name, lecithin; the systematic name is 1,2-diacyl-sn-glycero-3-phosphocholine); 3-sn-phosphatidylserine; 1-phosphatidylinositol [see comment (b) below]; 1,3-bis(3-sn-phosphatidyl)glycerol.

Comments. (a) It is understood that, in combination with compounds like ethanolamine (properly, 2-aminoethanol) or serine, which bear both hydroxyl and amino groups, substitution by phosphorus is at the hydroxyl group of the ethanolamine or serine. Substitution at any other position, or where confusion may arise, requires a locant.

(b) The phosphorylated derivatives of 1-(3-sn-phosphatidyl)inositol should be called 1-phosphatidylinositol 4-phosphate and 1-phosphatidylinositol 3,4-bisphosphate, respectively. The use of 'diphosphoinositide' and 'triphosphoinositide' for these is discouraged, as these names do not convey the chemical structures of the compounds and can be misleading. (Cf. also Table 4 in [10])

- Lip-2.5. As an alternative, generic names may be coined according to <u>Lip-1.13</u>, i.e. using glycerol phosphate (glycerophosphate) as the stem. In this case, the stereospecific numbering of glycerol should be used to indicate the position of the phosphoric residue as well as the other substituents (acyl-, alkyl-, 1-alkenyl). If the nature of these substituents cannot be specified, the prefix 'radyl' may be used.
- Lip-2.6. Derivatives of phosphatidic acids resulting from hydrolytic removal of one of the two acyl groups may be designated by the old prefix 'lyso', e.g. lysophosphatidylethanolamine for compound XIIb. A locant may be added to designate the site of (hydro)lysis, 2-lyso designating hydrolysis at position 2, leaving a free hydroxyl group at this carbon atom.

Comment. The 'lyso' term originated from the fact that these compounds are hemolytic. It is here redefined to indicate a limited hydrolysis of the phosphatidyl derivative (i.e. 'deacyl').

- Lip-2.7. The term 'plasmalogen' may be used as a generic term for glycerophospholipids in which the glycerol moiety bears an 1-alkenyl ether group.
- **Lip-2.8.** The term 'plasmenic acid' signifies a derivative of sn-glycero-3-phosphate in which carbon-1 bears an O-(l-alkenyl) residue, and position 2 is esterified with a fatty acid (XIII). This term can also be used to name derivatives, e.g. plasmenylethanolamine.

Comments. (a) The use of 'phosphatidyl' as a name for the acyl radical of phosphatidic acid has facilitated the nomenclature of its various compounds (see <u>Lip-2.4</u>). Therefore, it seems logical to offer a similar short term for XIII, i.e. 'plasmenic acid', as an alternative to the more systematic name, 2-acyl-1-alkenyl-sn-glycerol 3-phosphate, which, of course, may be used if desired. 'Plasmenic' is a contraction of 'plasmalogenic' and may be especially useful in naming derivatives, e.g., plasmenylserine.

(b) Isomers like those bearing the phosphate residue in position 2 (e.g. compound XIV) should not be named in this way but as derivatives of the corresponding glycerophosphate, using stereospecific numbering.

3-Acyl-1-(1-alkenyl)-sn-glycerol 2-phosphate

Lip-2.9. The term 'lysoplasmenic acid' may be used for a derivative of sn-glycero-3-phosphate that has an O-(1-alkenyl) residue on carbon-1, the hydroxyl group in position 2 being unsubstituted (XVa). This name may also be used in combinations like 'lysoplasmenylethanolamine' (XV b).

CH2O-CH=CH-R'

HOE-CH2O-CH=CH-R'

HOE-CH2O-PO(OH)-O-R"

XVa: 
$$(R'' = H)$$
: a lysoplasmenic acid

XVb:  $(R'' = CH_2CH_2NH_2)$  a lysoplasmenylethanolamine

Lip-2.10. For compounds of type XVI, bearing a saturated ether group in position 1 and an acyl group in position 2 of *sn*-glycero-3-phosphate, the term *'plasmanic acid'* is proposed. Compounds deacylated in position 2, or with a substituent on the phosphoric residue, can be treated as are the plasmenic acids (Lip-2.9).

Comment. The proposed names will be especially useful for naming phosphoric diesters (phosphodiesters), e.g., plasmanylethanolamine, instead of 2-acyl-1-alkyl-sn-glycero-3-phosphoethanolamine. The terms 'plasmanic acid' and 'plasmanyl' may also be applied to ethers with an alkyl group bearing a double bond within the chain, e.g. a 9-hexadecenyl residue (derived from palmitoleic acid). In such cases, the proper term 'alkenyl', if used without the 'ene' locant(s), would be misleading. (See Lip-1.17.)

## **B.** Individual Compounds

**Lip-2. 11.** Individual glycerophospholipids in which the substituents can be specified are named according to existing Rules [2, 3, 5, 6], using the infix '-phospho-' [2, 10] to indicate the phosphodiester bridge.

Example: 1-palmitoyl-2-stearoyl-sn-glycero-3-phosphoethanolamine for compound XVII.

CH<sub>2</sub>O-CO-C<sub>1</sub>
$$\neq$$
H<sub>51</sub>

C<sub>1</sub> $\neq$ H<sub>55</sub> -CO-O $\rightleftharpoons$ C $\rightleftharpoons$ H

CH<sub>2</sub>O-PO(OH)-OCH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub>

XVII

1-Palmitoyl-2-stearoyl-sn-glycero-3-phosphoethanolamine

Lip-2.12. The ketone derived from glycerol, 1,3-dihydroxy-2-propanone, also known as dihydroxyacetone, may be termed 'glycerone', if desired. The name is a contraction of 'glyceroketone' and may be useful to emphasize the relationship with glycerol, glyceraldehyde (glyceral), and glycerate. It also permits a simple symbolism (<u>Appendix B</u>) and the naming of derived lipids, e.g., 1-palmitoyl-3-phosphoglycerone.

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Continued with Recommendations Lip-3 and Lip-4

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#### Nomenclature of Lipids

## Recommendations Lip-3 and Lip-4

Continued from Lip-1 and Lip-2

#### Contents of this section

- III. Glycolipids
  - o A. General considerations
  - o B. Generic terms (Lip-3.1 to Lip-3.5)
  - o C. Individual compounds (Lip-3.6 to Lip-3.12)
  - o D. Symbols and abbreviations (Lip-3.13 to Lip-3.14)
- IV. Neuraminic acid (Lip-4.1 to Lip-4.3)
- References

#### III. GLYCOLIPIDS

#### A. General Considerations

Glycolipids (a contraction of glycosyllipids) are generally named as glycosyl derivatives of the corresponding lipid, e.g., diacylgalactosylglycerol, glucosylceramide. Because of the heterogeneity of the fatty acids and long-chain bases encountered in most cases, a generic name for the lipid moiety is needed, i.e. ceramide. With higher glycosphingolipids, especially the gangliosides, naming problems arise from the complexity of the carbohydrate moiety of these compounds. The systematic names of the oligosaccharides linked to ceramide are so cumbersome that they are of the same practical value as, e.g., the systematic name for a peptide hormone such as insulin. It was felt that this difficulty could be overcome only by creating suitable trivial names for some parent oligosaccharides. In constructing these names (see <u>Table 1</u>) the following principles were observed:

- (a) The number of monosaccharide units in an oligosaccharide is indicated by the suffixes '-biose', '-triaose', 'tetraose', etc. This follows the well established practice in the carbohydrate field (cf. cellobiose, cellotetraose, maltotetraose, etc.), with the exception that the suffix '-triose', as used in maltotriose, has been changed to 'triaose' to avoid confusion with the monosaccharides called trioses.
- (b) The oligosaccharides are grouped in series according to their structure and biogenetic relationship.
- (c) Differences in linkage (e.g.,  $1 \rightarrow 4$  versus  $1 \rightarrow 3$ ) in otherwise identical sequences are indicated by 'iso- 'or 'neo-', used as a prefix. On the basis of these names, the semisystematic nomenclature for neutral glycosphingolipids and gangliosides described below is recommended. A set of symbols has been devised that allows a simple representation of complex neutral and acidic glycosphingolipids (<u>Table 1</u>).

Table 1. Names and abbreviations of simple glycolipids

G	Trivial name of	~	Short
Structure*	oligosaccharide <sup>b</sup>	Symbol <sup>c</sup>	symbol <sup>d</sup>

Gal(α1-4)Gal(β1-4)GlcCer	Globotriaose	GbOse <sub>3</sub>	$Gb_3$
GalNAc( $\beta$ 1-3)Gal( $\alpha$ 1-4)Gal( $\beta$ 1-4) GlcCer	Globotetraose	GbOse <sub>4</sub>	$\mathrm{Gb}_{4}$
Gal(α1-3)Gal(β1-4)GlcCer	Isoglobotriaose	iGbOse <sub>3</sub>	$iGb_3$
GalNAc( $\beta$ 1-3)Gal( $\alpha$ 1-3)Gal( $\beta$ 1-4) GlcCer	Isoglobotetraose	iGbOse <sub>4</sub>	iGb <sub>4</sub>
Gal(β1-4)Gal(β1-4)GlcCer	Mucotriaose	McOse <sub>3</sub>	$Mc_3$
Gal(β1-3)Gal(β1-4)Gal(β1-4)GlcCer	Mucotetraose	McOse <sub>4</sub>	$Mc_4$
GlcNAc(β1-3)Gal(β1-4)GlcCer	Lactotriaose	LcOse <sub>3</sub>	$Lc_3$
Gal(β1-3)GlcNAc(β1-3)Gal(β1-4) GlcCer	Lactotetraose	LcOse <sub>4</sub>	Lc <sub>4</sub>
Gal(β1-4)GlcNAc(β1-3)Gal(β1-4) GlcCer	Neolactotetraose	nLcOse <sub>4</sub>	nLc
GalNAc(β1-4)Gal(β1-4)GlcCer	Gangliotriaose	GgOse <sub>3</sub>	$Gg_3$
Gal(β1-3)GalNAc(β1-4)Gal(β1-4) GilcCer	Gangliotetraose	$\mathrm{GgOse}_4$	$Gg_4$
Gal(α1-4)GalCer	Galabiose	GaOse <sub>2</sub>	$Ga_2$
Gal(1-4)Gal(α1-4)GalCer	Galatriaose	GaOse <sub>3</sub>	$Ga_3$
GalNAc(1-3)Gal(1-4)Gal(α1-4) GalCer	N-Acetylgalactosaminylgalatriaose	GalNAc1- 3GaOse <sub>3</sub>	-

<sup>&</sup>lt;sup>a</sup> Symbols and arrangement are discussed in <u>Lip-3.13</u>. Hyphens replace left-to-right arrows (see Section 3.4 of [13]).

#### B. Generic Terms

Lip-3.1. The term 'glycolipid' designates any compound containing one or more monosaccharide residues linked by a glycosyl linkage to a lipid part [e.g., a mono- or diacylglycerol, a long-chain base (sphingoid) like sphingosine, or a ceramide].

Lip-3.2. The term 'glycoglycerolipid' may be used to designate glycolipids containing one or more glycerol residues.

Lip-3.3. The term 'glycosphingolipid', as hitherto, includes all compounds containing at least one monosaccharide and a sphingoid. The glycosphingolipids can be subdivided as follows:

Neutral glycosphingolipids: monoglycosyl- and oligoglycosylsphingoids; monoglycosyl- and

<sup>&</sup>lt;sup>b</sup> Name of glycolipid is formed by converting ending '-ose' to '-osyl', followed by '-ceramide', without space; e.g., globotriaosylceramide.

<sup>&</sup>lt;sup>c</sup> Should be followed by Cer for the glycolipid, without space; e.g., McOse<sub>3</sub>Cer, Mc<sub>4</sub>Cer (see <u>Lip-3.13</u>).

<sup>&</sup>lt;sup>d</sup> The short form should be used only in situations of limited space or in case of frequent repetition.

oligoglycosylceramides.

Acidic glycosphingolipids: sialosy1glycosylsphingolipids (gangliosides); sulfoglycosylsphingolipids (formerly 'sulfatides', which is not recommended) (cf. <u>Lip-3.11</u>).

Lip-3.4. 'Psychosine' may be used as a generic name for 1-monoglycosylsphingoids, although the latter is preferred. The nature of the monosaccharide and the sphingoid is not specified in this name.

Lip-3.5. The term 'fucolipid' may be used to designate fucose-containing neutral or acid glycolipids.

### C. Individual Compounds

Note. 'Individual' in this section refers to the carbohydrate moiety only.

Lip-3.6. Glycoglycerolipids may be named either as glycosyl compounds according to Rule Carb-24 or as glycosides according to Rule Carb-23 [5].

Example: the compound XVIII may be named either 1,2-diacyl-3- $\beta$ -D-galactosyl-sn-glycerol or 1,2-diacyl-sn-glycerol 3- $\beta$ -D-galactoside.

Comment. The first form is preferred, as the glycosphingolipids are also named this way.

Lip-3.7. A glycosphingolipid is generally named as a 'glycosylsphingoid' or a 'glycosylceramide', using the appropriate trivial name of the mono- or oligosaccharide residue for 'glycosyl'. It is understood that the sugar residue is attached to the C-1 hydroxyl group of the ceramide. For glycosphingolipids carrying two to four saccharide residues, the trivial names listed in Table 1 are recommended.

**XVIII** 

Comment. It is strongly recommended that the name of the oligosaccharide be defined in each publication by means of the standard symbols for sugars (as in Table 1, column 1) rather than by the full name, which is often so long as to be confusing.

Lip-3.8. The trivial name 'cerebroside' designates 1- $\beta$ -glycosylceramide (the natures of the sphingoid and of the fatty acid are not specified in this name).

Lip-3.9. Glycosphingolipids carrying fucose either as a branch or at the end of an oligohexosyleeramide are named as 'fucosyl(X)osylceramide' where (X) stands for the root name of the oligosaccharide. The location of the fucosyl residue is indicated by a Roman numeral designating the position of the

monosaccharide residue in the parent oligosaccharide (counting from the ceramide end) to which the fucose residue is attached, with an Arabic numeral superscript indicating the position within that residue to which the fucose is attached. If necessary, the anomeric symbol can be used as usual, i.e. preceding 'fucosyl-'.

Examples for <u>Lip-3.7</u> and <u>Lip-3.9</u> (structures given in the symbols of <u>Lip-3.13</u>):

- (a) lactosylceramide for Gal  $(\beta 1 \rightarrow 4)$ GlcCer;
- (b) mucotriaosylceramide for  $Gal(\beta 1 \rightarrow 4)Gal(\beta 1 \rightarrow 4)GlcCer$ ;
- (c) III<sup>2</sup>- $\alpha$ -fucosylisoglobotriaosylceramide for Fuc( $\alpha$ 1 $\rightarrow$ 2)Gal( $\alpha$ 1 $\rightarrow$ 3)Gal( $\beta$ 1 $\rightarrow$ 4)Glc( $\beta$ 1 $\rightarrow$ 1)Cer.

Note. D is omitted by convention in the abbreviated formulas, but D (or L) may be inserted when desirable. Hyphens may replace left-to-right arrows (see section 3.4 of [13]).

Lip-3.10. Sialoglycosphingolipids (synonym: gangliosides) are glycosphingolipids carrying one or more sialic residues. Sialic acid is the generic term for N-acetyl- or N-glycoloylneuraminic acid (cf. section 3 in [1]). Gangliosides are named as N-acetyl- (or N-glycoloyl-)neuraminosyl-(X)osylceramide, where (X) stands for the root name of the neutral oligosaccharide to which the sialosyl residue is attached (cf. Table 1). The position of the sialosyl residue is indicated in the same way as in the case of fucolipids (see Lip-3.9).

Example: II<sup>3</sup>-N-acetylneuraminosyllactosylceramide for AcNeu( $\alpha 2 \rightarrow 3$ )Gal( $\beta 1 \rightarrow 4$ )Glc( $\beta 1 \rightarrow 1$ )Cer.

Lip-3.11. Glycosphingolipids carrying a sulfuric ester (sulfate) group, formerly called sulfatides, are preferably named as sulfates of the parent neutral glycosphingolipid. The location of the sulfate group may be indicated as in <u>Lip-3.9</u>.

Example: lactosylceramide II<sup>3</sup>-sulfate.

Lip-3.12. Phosphoglycosphingolipids with phosphodiester structures are named according to the recommendation for the phospholipids (see above).

Neuraminic acid
5-amino-3,5-dideoxy-D-glycero-D-galacto-nonulopyra nosonic acid
(a) (b)

#### D. Symbols and Abbreviations

Lip-3.13. Simple or complex glycosphingolipids can be represented according to existing rules, using the symbols Cer, Sph, AcNeu, etc. (Appendix B), together with the recommended [13] symbols for the hexoses (Glc, Gal, etc.). Examples are given above, and in Table 1 and Appendix C. However, due to the complexity of the higher glycosphingolipids, this often results in very long and cumbersome series that are not easy to comprehend. It is therefore recommended that the oligosaccharides listed in Table 1 be represented by specific symbols in which the number of monosaccharide units (-oses) is indicated by Osen, preceded by two letters representing the trivial name of the oligosaccharide (column 3). For a short form, which may be required in the case of limited space or frequent repetition, Ose can be omitted (column 4); however, the long form is preferred as being more evocative.

#### Examples:

- (a) McOse<sub>3</sub>Cer for mucotriaosylceramide,  $Gal(\beta 1-4)Gal(\beta 1-4)Glc(1-1)Cer$ ;
- (b) II<sup>3</sup> AcNeuGgOse<sub>4</sub>Cer for II<sup>3</sup>-N-acetylneuraminosylgangliotetraosylceramide, Gal $\beta$ 1  $\rightarrow$ 3GalNAc $\beta$ 1  $\rightarrow$ 4Gal(3  $\leftarrow$ 2- $\alpha$ NeuAc) $\beta$ 1  $\rightarrow$ 4Glc $\beta$ 1  $\rightarrow$ 1Cer (see <u>Lip-3.14</u> for this mode of representing a branched chain).

Abbreviations for the more important gangliosides are given in Appendix C.

Lip-3.14. When it is desirable to represent a branched oligosaccharide on a single line, as in running text or a table, the parentheses surrounding the locants in the main chain may be omitted and used instead to enclose the symbols for the branched portion(s) of the molecule. The branches follow, in parentheses and with appropriate arrows, the residues to which they are attached.

## Examples:

- (a) NeuGc $\alpha$ 2 $\rightarrow$ 3Gal $\beta$ 1 $\rightarrow$ 3GalNAc $\beta$ 1 $\rightarrow$ 4Gal(3 $\leftarrow$ 2 $\alpha$ NeuGc) $\beta$ 1 $\rightarrow$ 4Glc $\beta$ 1 $\rightarrow$ 1Cer;
- (b) NeuAc $\alpha$ 2 $\rightarrow$ 3Gal $\beta$ 1 $\rightarrow$ 3GalNAc $\beta$ 1 $\rightarrow$ 4Gal(3 $\leftarrow$ 2 $\alpha$ NeuAc8 $\leftarrow$ 2 $\alpha$ NeuAc) $\beta$ 1 $\rightarrow$ 4Glc $\beta$ 1 $\rightarrow$ 1Cer;
- (c) GalNAc $\alpha$ 1g $\rightarrow$ 3Gal(2 $\leftarrow$ 1 $\alpha$ Fuc) $\beta$ 1 $\rightarrow$ 4GlcNAc(3 $\leftarrow$ 1 $\alpha$ Fuc) $\beta$ 1 $\rightarrow$ 3Gal $\beta$ 1 $\rightarrow$ 4Glc $\beta$ 1 $\rightarrow$ 1Cer  $\equiv$  III<sup>3</sup>,IV<sup>2</sup>- $\alpha$ , $\alpha$ -difucosyl-IV<sup>3</sup>- $\alpha$ -2-acetamido-2-deoxgalactosylneolactotetraosylceramide  $\equiv$  III<sup>3</sup>,IV<sup>2</sup> (Fuc $\alpha$ )<sub>2</sub>,IV<sup>3</sup>GalNAca-nLcOse<sub>4</sub>Cer.

#### IV. NEURAMINIC ACID

- Lip-4.1. The compound 5-amino-3,5-dideoxy-D-glycero-D-galacto-nonulosonic acid is neuraminic acid (XIX), with the symbol Neu [11].
- Lip-4.2. The term 'sialic acid' signifies the *N*-acylneuraminic acids and their esters and other derivatives of the alcoholic hydroxyl groups.
- Lip-4.3. The radicals resulting from the removal of a hydroxyl group of neuraminic acid or sialic acid are designated as neuraminoyl or sialoyl, respectively, if the hydroxyl is removed from the carboxyl group, and as neuraminosyl and sialosyl, respectively, if the hydroxyl group is removed from the anomeric carbon atom of the cyclic structure.

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- 13. IUPAC-IUB Combined Commission on Biochemical Nomenclature (1967) Eur. J. Biochem. 1, 259-266 [see also Bull. Soc. Chim. Biol. 50, 3-20 (1968) (in French)].

Continued with Appendixes A-C

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## Nomenclature of Lipids

## Appendixes A-C

## Continued from Lip-3 and Lip-4

### Contents of this section

- Appendix A: names of and symbols for higher fatty acids
- Appendix B: symbols recommended for various constituents of lipids
- Appendix C: abbreviated representation of gangliosides

## Appendix A. Names of and symbols for higher fatty acids

Nun	nerical symbol	Structure	Stems o	f	'Name'
		$H_3C-(R)-CO_2H$	systematic names <sup>a</sup>	trivial names <sup>b</sup>	symbol
1	10:0	-[CH <sub>2</sub> ] <sub>8</sub> -	Decano-	Capr- <sup>c</sup>	Dec
2	12:0	-[CH <sub>2</sub> ] <sub>10</sub> -	Dodecano-	Laur-	Lau
3	14:0	-[CH <sub>2</sub> ] <sub>12</sub> -	Tetradecano-	Myrist-	Myr
4	16:0	-[CH <sub>2</sub> ] <sub>14</sub> -	Hexadecano-	Palmit-	Pam
5	16:1	-[CH2]5CH=CH[CH2]7-	9-Hexadeceno-	Palmitole-	ΔPam
6	18:0	-[CH <sub>2</sub> ] <sub>16</sub> -	Octadecano-	Stear-	Ste
7	18:1(9)	-[CH2]7CH=CH[CH2]7-	cis-9-Octadeceno-	Ole-	Ole
8	18:1(11)	-[CH2]5CH=CH[CH2]9-	11-Octadeceno-	Vaccen-	Vac
9	18:2(9,12)	-[CH <sub>2</sub> ] <sub>3</sub> (CH <sub>2</sub> CH=CH) <sub>2</sub> [CH <sub>2</sub> ]	cis, cis-9,12- Octadecadieno-	Linole	Lin
10	18:3(9,12,15)	$-(\mathrm{CH_2CH=CH)_3[CH_2]_7}-$	9,12,15-Octadecatrieno-	(9,12,15)- Linolen-	$\alpha Lnn$
11	18:3(6,9,12)	-[CH <sub>2</sub> ] <sub>3</sub> (CH <sub>2</sub> CH=CH) <sub>3</sub> [CH <sub>2</sub> ] <sub>4</sub> -	6,9,12-Octadecatrieno-	(6,9,12)-Linolen-	γLnn
12	18:3(9,11,13)	$-[CH_2]_3(CH=CH)_3[CH_2]_7$	9,11,13-Octadecatrieno-	Eleostear-	eSte
13	20:0	-[CH <sub>2</sub> ] <sub>18</sub> -	Icosano-d	Arachid-	Ach
14	20:2(8,11)	-[CH <sub>2</sub> ] <sub>6</sub> (CH <sub>2</sub> CH=CH) <sub>2</sub> [CH <sub>2</sub> ]	8,11-Icosadieno-d		$\Delta_2$ Ach
15	20:3(5,8,11)	-[CH <sub>2</sub> ] <sub>6</sub> (CH <sub>2</sub> CH=CH) <sub>3</sub> [CH <sub>2</sub> ] <sub>3</sub>	5,8,11-Icosatrieno-d	,	$\Delta_3$ Ach
16	20:4	-[CH <sub>2</sub> ] <sub>3</sub> (CH <sub>2</sub> CH=CH) <sub>4</sub> [CH <sub>2</sub> ]	5,8,11,14-Icosatetraeno-d	Arachidon-	$\Delta_4$ Ach

	(5,8,11,14)	3			
17	22:0	-[CH <sub>2</sub> ] <sub>20</sub> -	Docosano-	Behen-	Beh
18	24:0	-[CH <sub>2</sub> ] <sub>22</sub> -	Tetracosano-	Lignocer-	Lig
19	24:1	$-[\mathrm{CH_2}]_7\mathrm{CH} = \mathrm{CH}[\mathrm{CH_2}]_{13}-$	cis-15-Tetracoseno-	Nervon-	Ner
20	26:0	$[CH_2]_{24}$ -	Hexacosano-	Cerot-	Crt
21	28:0	-[CH <sub>2</sub> ] <sub>26</sub> -	Octacosano-	Montan-	Mon

<sup>&</sup>lt;sup>a</sup> Ending in '-ic', '-ate', '-yl', for acid, salt or ester, acyl radical, respectively.

## Appendix B. Symbols recommended for various constituents of lipids

Name	Symbol <sup>a</sup>
For alkyl radicals <sup>b</sup>	R
Methyl, ethyl, dodecyl	Me, Et, Pr, Bu, Pe, Hx, Hp, Oc, Nn, Dec, Und, Dod
For aliphatic carboxylic acids <sup>b</sup>	Acyl (not abbreviated), RCO-
Formyl, acetyl, glycoloyl, propionyl	Fo (or HCO), Ac, Gc, Pp
Butyryl, valeryl	Br, Vl
Hexanoyl, heptanoyl, octanoyl	Hxo, Hpo, Oco
Nonanoyl, decanoyl, undecanoyl	Nno, Dco, Udo
Lauroyl, myristoyl, palmitoyl	Lau, Myr, Pam
Stearoyl, eleostearoyl, linoleoyl, arachidonoyl	Ste, eSte, Lin, $\Delta_4$ Ach
For glycerol and its oxidation products <sup>c</sup>	
Glycerol, glyceraldehyde, glycerone, glyceric acid	Gro, Gra, Grn, Gri
For 'glycosyl'	Ose
Glucose, galactose, fucose	Glc <sup>d</sup> , Gal, Fuc
Gluconic acid, glucuronic acid	GlcA, GlcU <sup>e</sup>
Glucosamine <sup>f</sup> , N-acetylglucosamine	GlcN, GlcNAc
Neuraminic, sialic, muramic acids	Neu, Sia, Mur
N-Acetylneuraminic acid, N-glycoloylneuraminic acid	d NeuAc <sup>g</sup> , NeuGc
Deoxy	d
Miscellaneous	
Ceramide, choline, ethanolamine	Cer, Cho, Etn <sup>h</sup>
Inositol, serine	Ins, Ser
Phosphatidyl, sphingosine, sphingoid, Phosphoric residue	Ptd, Sph, Spd, P
3.T1 1.1 1.1 1.1 1.1 1.1 1.1 1.1 1.1 1.1	1

<sup>&</sup>lt;sup>a</sup> These symbols are constructed in analogy to those already in use for amino acids and saccharides [11, 13]; they may assist the abbreviated representation of more complex lipids in a way similar to the

<sup>&</sup>lt;sup>b</sup> Ending in '-ic', '-ate', '-oyl' for acid, salt or ester, or acyl radical, respectively.

<sup>&</sup>lt;sup>c</sup> Not recommended because of confusion with caproic (hexanoic) and caprylic (octanoic) acids. Decanoic is preferred.

<sup>&</sup>lt;sup>d</sup> Formerly 'eicosa' (Changed by IUPAC Commission on Nomenclature of Organic Chemistry, 1975).

peptides and polysaccharides. Prefixes such as 'iso-', 'tert-', 'cyclo' are specified in the symbols by lower-case superscripts ( $Pr^i$ ,  $Bu^t$ ,  $Hx^c$ ) or lower-case prefixes (iPr, tBu, cHx), unsaturation by, e.g.,  $\Delta^3$  for a 3,4 double bond,  $\Delta^3$  for a 3,4 triple bond (cf. Proteins, Vol. I, pp. 96-108, in *Handbook of Biochemistry*, 3rd edition, edited by G. Fasman, CRC Press, Cleveland, Ohio, 1976). Many of these symbols are drawn from previously published Recommendations [11, 12]. See also Appendix A.

## Appendix C. Abbreviated representation of gangliosides

Lipid Document <sup>a</sup>	Designation according to Wiegand	t <sup>b</sup> Svennerholm <sup>c</sup>
1. I <sup>3</sup> NeuAc-GalCer	G <sub>Gal</sub> 1NeuAc	-
2. II <sup>3</sup> NeuAc-LacCer	G <sub>Lac</sub> 1NeuAc	$G_{M3}$
3. II <sup>3</sup> NeuGe-LacCer	G <sub>Lac</sub> 1NeuNGl	-
4. II <sup>3</sup> (NeuAc) <sub>2</sub> -LacCer	G <sub>Lac</sub> 2NeuAc	$G_{D3}$
5. II <sup>3</sup> NeuAc/NeuGc-LacCer	G <sub>Lac</sub> 2NeuAc/NeuNGl	-
6. II <sup>3</sup> NeuGc-LacCer	G <sub>Lac</sub> 2NeuNGl	-
7. II <sup>3</sup> NeuAc-GgOse <sub>3</sub> Cer	G <sub>Gtri</sub> 1NeuAc	$G_{M2}$
8. II <sup>3</sup> NeuAc-GgOse <sub>4</sub> Cer	G <sub>Gtet</sub> 1NeuAc	$G_{M1}$
9. IV <sup>3</sup> NeuAc-nLcOse <sub>4</sub> Cer	G <sub>Lntet</sub> laNeuAc	$G_{ ext{M1-GlcNAc}}$
10. IV <sup>6</sup> NeuAc-nLcOse <sub>4</sub> Cer	G <sub>Lntet</sub> 1bNeuAc	-
11. IV <sup>2</sup> Fuc,II <sup>3</sup> NeuAc-GgOse <sub>4</sub> Cer	G <sub>Gfpt</sub> 1NeuAc	-
12. IV <sup>3</sup> NeuAc-nLcOse <sub>4</sub> Cer	-	-
13.		

<sup>&</sup>lt;sup>b</sup> Systematic and recommended trivial names of unbranched, acyclic compounds only (cf. Appendix A). Other forms are created by prefixes (e.g., 'iso-', 'tert-', 'cyclo-'). See Appendix A.

<sup>&</sup>lt;sup>c</sup> These symbols form a self-consistent series for a group of closely related compounds. It is recognized that other abbreviations (but no symbols) are currently in use. (See <u>Lip-2.12.</u>)

<sup>&</sup>lt;sup>d</sup> Not Glu (glutamic acid) or G (nonspecific).

<sup>&</sup>lt;sup>e</sup> Recommended in place of GlcUA, the 'A' being unnecessary.

f Approved trivial name for 2-amino-2-deoxyglucose; similarly for galactose (GalNAc), etc.

<sup>&</sup>lt;sup>g</sup> AcNeu was recommended earlier [11]. When it is necessary to differentiate between N-acetyl and O-acetyl derivatives, NeuNAc and NeuOAc (italicized locants, in contradistinction to GalNAc, etc.) may be employed.

<sup>&</sup>lt;sup>h</sup> May take the form OEtN< if substitution on the nitrogen atom is to be indicated.

II <sup>3</sup> (NeuAc) <sub>2</sub> -GgOse <sub>4</sub> Cer	G <sub>Gtet</sub> 2bNeuAc	$G_{D1b}$
14. IV <sup>3</sup> NeuAc,II <sup>3</sup> NeuAc-GgOse <sub>4</sub> Cer	G <sub>Gtet</sub> 2aNeuAc	$G_{D1a}$
15. II <sup>3</sup> (NeuAc)3-GgOse <sub>4</sub> Cer	G <sub>Gtet</sub> 3bNeuAc	-
16. IV <sup>3</sup> NeuAc,II <sup>3</sup> (NeuAc) <sub>2</sub> -GgOse <sub>4</sub> Cer	G <sub>Gtet</sub> 3aNeuAc	$G_{T1}$
17. IV <sup>3</sup> NeuAc,II <sup>3</sup> (NeuAc) <sub>3</sub> -GgOse <sub>4</sub> Cer	G <sub>Gtet</sub> 4bNeuAc	-
18. IV <sup>3</sup> (NeuAc) <sub>2</sub> II <sup>3</sup> (NeuAc) <sub>3</sub> -GgOse <sub>4</sub> Cer	G <sub>Gtet</sub> 5NeuAc	-
19. IV <sup>3</sup> NeuAc,II <sup>3</sup> NeuAc-GgOse <sub>5</sub> Cer	G <sub>Gpt</sub> 2aNeuAc	-

<sup>&</sup>lt;sup>a</sup> To indicate linkage points and anomeric form: Fuc should be written ( $\leftarrow 1\alpha$ Fuc); NeuAc should be written ( $\leftarrow 2\alpha$ NeuAc); (NeuAc)<sub>2</sub> should be written ( $\leftarrow 2\alpha$ NeuAc8)<sub>2</sub>; etc. If these features are assumed or defined, the short form used in this column is more convenient for use in texts and tables.

Continued with Supplement: derivatives of phosphatidic acid

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<sup>&</sup>lt;sup>b</sup> The subscripts to G (for ganglioside), from 7 on, have the meanings: Gtri = gangliotriose, Gtet = gangliotetraose, Litet = lactoisotetraose, Gpt = gangliopentaose, Gfpt = gangliofucopentaose [Wiegand, H. (1973) *Hoppe-Seyler's Z. Physiol. Chem.* **354**, 1049].

<sup>&</sup>lt;sup>c</sup> G = ganglioside, M = monosialo, D = disialo, T = trisialo. Arabic numerals indicate sequence of migration in thin-layer chromatograms [Svennerholm, L. (1963) *J. Neurochem.* 10, 613].



## Supplement: Derivatives of phosphatidic acid

### Continued from Appendixes A-C

From the JCBN/NC-IUB Newsletter 1980 (ref 14)

The 1976 recommendations [Compendium, pp. 122-132; see also Eur. J. Biochem. 79 (1977) 11-21(ref 15)] emphasized generic names for common lipids, names based on the stem name phosphatidic acid. In the light of recent interest in membrane lipids and of progress in both isolation and chemical synthesis of individual glycerophospholipids, it seems desirable to specify more exactly how individual compounds may be named.

According to the published recommendations (<u>Lip-2.11</u>), glycerophospholipids with known acyl residues are named as the acyl derivatives of glycerophosphocholine, glycerophosphoethanolamine. Thus, the following compound

$$\begin{array}{ccc} & \text{CH}_2\text{-O-CO-[CH}_2]_{14}\text{-CH}_9\\ \text{H}_9\text{C-[CH}_2]_{14}\text{-CO-O-CH} & \text{O}\\ & \text{CH}_2\text{-O-P-O-CH}_2\text{-CH}_2\text{-N(CH}_9)_9\\ & \text{CH}_2\text{-O-P-O-CH}_2\text{-CH}_2\text{-N(CH}_9)_9\\ & \text{O-} \end{array}$$

is called dipalmitoylglycerophosphocholine (dihexadecanoylglycerophosphocholine). For abbreviated nomenclature, the system using three-letter symbols given in Appendix B of the published document may be used. Thus the compound may be written as: Pam<sub>2</sub>Gro-*P*-Cho.

Comment. This compound has sometimes been incorrectly called dipalmitoyl lecithin. But lecithin, like the recommended term phosphatidylcholine, already contains two (unspecified) acyl groups, so such a name could imply the presence of two more acyl groups. Similarly glycerophospholipids with a high content of polyene acids may be termed polyenoylglycerophosphocholines if desired, but not polyenoylphosphatidylcholines.

The 'Compendium' mentioned in the first line of this note is the preceding edition of Biochemical nomenclature and related documents, The Biochemical Society, London 1978 [now as a second edition 1992 (ref 16)].

#### References

- 14. IUPAC-IUB Joint Commission on Biochemical Nomenclature (JCBN), and Nomenclature Commission of IUB (NC-IUB). Newsletter 1980, Eur. J. Biochem., 1980, 104, 321-322; Hoppe-Seyler's Z. Physiol. Chem., 1980, 361, I-IV.
- 15. IUPAC-IUB Commission on Biochemical Nomenclature (CBN), Nomenclature of lipids (1976), Biochem. J., 1978, 171, 21-35; Chem. Phys. Lipids, 1978, 21, 159-173; Eur. J. Biochem., 1977, 79, 11-21; Hoppe-Seyler's Z. Physiol. Chem., 1977, 358, 617-631; J. Lipid Res., 1978, 19, 114-128; Lipids, 1977, 12, 455-468; Mol. Cell. Biochem., 1977, 17, 157-171; Biochemical Nomenclature and Related

Documents, 2nd edition, Portland Press, 1992, pages 180-190.

**16.** International Union of Biochemistry and Molecular Biology, <u>Biochemical Nomenclature and Related Documents</u>, 2nd edition, Portland Press, 1992, Edited by C Liébecq.

Continued with <u>Lip-1.10</u> - no longer recommended.

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#### Nomenclature of Lipids

## No Longer Recommended

## Lip-1.10

## Continued from suplement

The recommendations on the <u>Nomenclature of Glycolipids</u> imply that parts of Lip-1.10 are no longer recommended. The following is the full original text. As a consequence some alternative names quoted elsewhere in the document have been omitted from the web version. These too are listed below.

Lip-1.10. Affixes denoting substitution of sphinganine (hydroxy, oxo, methyl, etc.) are used as usual, according to existing rules [3]. The configurations of additional substituents should be specified by the prefixes 'D' or 'L' (italic capitals, cf. [4]), following the locant of substitution. These prefixes refer to the orientation of the functional groups to the right or left, respectively, of the carbon chain when written vertically in a Fischer projection with C-1 at the top (cf. Formulae I-VI). If the configuration is unknown, the prefix 'X' may be used. In the case of a racemic mixture, 'rac' should be used as a prefix to the name.

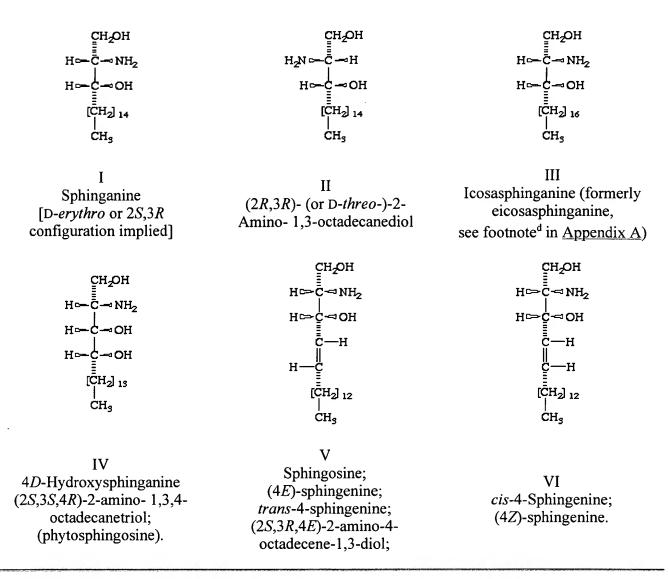
Sphingoids differing from sphinganine in their configurations at C-2 and/or C-3 should be named not as derivatives of sphinganine, but with fully systematic names [3], using the prefixes D-threo, L-erythro, as appropriate, e.g., D-threo-2-amino-1,3-octadecanediol, or (2R,3R)-2-amino-1,3-octadecanediol, for II (cf. Rule Carb-8 in [5]). (Cf. Lip-1.11, example [d]).

Comments. (a) The semisystematic names for the sphingoids are significantly shorter than the fully systematic names only if the terms chosen imply not only substituents but also configurations. Therefore, the name 'sphinganine' specifies the D-erythro configuration, and it is logical that the names of stereoisomers of sphinganine differing in configuration at C-2 and/or C-3 should not include 'sphinganine' as a root. This recommendation differs from that in the previous document [1].

(b) The configurations usually encountered have identical configurational prefixes only if a D/L but not if the R/S system [6] is used; e.g., C-3 is D and R in icosasphinganine (III) and D and S in AD-hydroxysphinganine (IV). Whenever it is desirable to use the R/S system, the fully systematic name should be used with the specification of configuration at every center (and, when applicable, of the configuration at the double bond).

#### Examples:

- (a) (2R,3R)-2-amino-1,3-octadecanediol, for II;
- (b) (2S,3S,4R)-2-amino-1,3,4-octadecanetriol for IV;
- (c) (2S,3R,4E)-2-amino-4-octadecene-1,3-diol for sphingosine (V) (See also Lip-1.11).



The following names have been omitted from the web version:

IV was also called 4D-Hydroxysphinganine (as above but omitted from the main web version of the lipid document).

Lip-1.8 spinganine was also called 2D-amino-1,3D-octadecanediol.

Lip-1.11 last paragraph, example (a) read: 4D-hydroxysphinganine for IV, formerly known as phytosphingosine;

#### References for this section

- 1. IUPAC-IUB Commission on Biochemical Nomenclature (1967) Eur. J. Biochem. 2, 127-131, also 12, 1 (1970); [see also Biochemistry, 6, 3287-3292 (1967); Biochem. J., 105, 897-902 (1967); J. Biol. Chem., 242, 4845-4849 (1967); Hoppe-Seyler's Z. Physiol. Chem., 350, 279-285 (1969) (in German)].
- 3. International Union of Biochemistry (1966) Nomenclature of Organic Chemistry (Sections A, B and C) 2nd edn, Butterworths, London. [See also Nomenclature of Organic Chemistry, Sections A, B, C, D.

- E, F, and H, Pergamon Press, 1979. Edited by J Rigaudy and S P Klesney.]
- 4. Mills, J. A. & Klyne, W. (1954) Progr. Stereochem. 1, 181.
- **5.** IUPAC Commission on the Nomenclature of Organic Chemistry and IUPAC-IUB Commission on Biochemical Nomenclature (1971) *Eur. J. Biochem.* **21**, 455-477, also **25**, 4 (1972) [now revised as Nomenclature of Carbohydrates (1996) Carb-15 is now 2-Carb-24.1].
- 6. International Union of Pure and Applied Chemistry (1970) J. Org. Chem. 35, 2849-2867; also Eur. J. Biochem. 18, 151-170 (1971) [now revised as Nomenclature of Organic Chemistry: Section E].

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